Computing f(A)b for Matrix Functions f

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Includes joint work with Philip Davies.

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Outline

1. Definition of $f(A)$
2. $f(A)\,b$
   - Applications
   - Interpolation
   - Cauchy Integral
   - $\log(A)\,b$
   - $A^\alpha\,b$

Multiplicity of Definitions

There have been proposed in the literature since 1880
eight distinct definitions *of a matric function,*
by Weyr, Sylvester and Buchheim,
Giorgi, Cartan, Fantappiè, Cipolla,
Schwerdtfeger and Richter.

— **R. F. Rinehart,**
The Equivalence of Definitions of a Matric Function,
Amer. Math. Monthly (1955)

Jordan Canonical Form

$$Z^{-1}AZ = J = \mathrm{diag}(J_1, \dots, J_p), \qquad \underbrace{J_k}_{m_k \times m_k} = \begin{bmatrix} \lambda_k & 1 & & \\ & \lambda_k & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_k \end{bmatrix}$$

Definition

$$f(A) = Zf(J)Z^{-1} = Z\mathrm{diag}(f(J_k))Z^{-1},$$

$$f(J_k) = \begin{bmatrix} f(\lambda_k) & f'(\lambda_k) & \dots & \dfrac{f^{(m_k-1)}(\lambda_k)}{(m_k-1)!} \\ & f(\lambda_k) & \ddots & \vdots \\ & & \ddots & f'(\lambda_k) \\ & & & f(\lambda_k) \end{bmatrix}.$$

The Formula for $f(J_k)$

Write $J_k = \lambda_k I + E_k \in \mathbb{C}^{m_k \times m_k}$. For $m_k = 3$ we have

$$E_k = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \quad E_k^2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad E_k^3 = 0.$$

Assume f has Taylor expansion

$$f(t) = f(\lambda_k) + f'(\lambda_k)(t - \lambda_k) + \cdots + \frac{f^{(j)}(\lambda_k)(t - \lambda_k)^j}{j!} + \cdots .$$

Then

$$f(J_k) = f(\lambda_k)I + f'(\lambda_k)E_k + \cdots + \frac{f^{(m_k-1)}(\lambda_k)E_k^{m_k-1}}{(m_k-1)!}.$$

Interpolation (1)

Definition (Sylvester, 1883; Buchheim, 1886)

Distinct e'vals $\lambda_1, \ldots, \lambda_s$, $n_i =$ max size of Jordan blocks for λ_i. Then $f(A) = r(A)$, where r is unique Hermite interpolating poly of degree $< \sum_{i=1}^{s} n_i$ satisfying

$$r^{(j)}(\lambda_i) = f^{(j)}(\lambda_i), \qquad j = 0\colon n_i - 1, \quad i = 1\colon s.$$

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Example. Let $f(t) = t^{1/2}$, $A = \begin{bmatrix} 2 & 2 \\ 1 & 3 \end{bmatrix}$, $\lambda(A) = \{1, 4\}$.

Taking +ve square roots,

$$r(t) = f(1)\frac{t-4}{1-4} + f(4)\frac{t-1}{4-1} = \frac{1}{3}(t+2).$$

$$\Rightarrow \quad A^{1/2} = r(A) = \frac{1}{3}(A + 2I) = \frac{1}{3}\begin{bmatrix} 4 & 2 \\ 1 & 5 \end{bmatrix}.$$

Interpolation (2)

Properties

- $f(A) = r(A)$ is a polynomial in A.
- Poly r **depends on A**.
- This def. **preserves functional relations** $G(f_1, \ldots, f_p) = 0$, where G is a polynomial. E.g.
  - $\sin^2(A) + \cos^2(A) = I$,
  - $(A^{1/p})^p = A$,
  - $e^{iA} = \cos A + i \sin A$.

But of course $e^{A+B} \neq e^A e^B$.

Cauchy Integral Theorem

Definition

$$f(A) = \frac{1}{2\pi i} \int_{\Gamma} f(z)(zI - A)^{-1}\, dz,$$

where f is analytic on and inside a closed contour Γ that encloses $\lambda(A)$.

Equivalence of Definitions

The three definitions are **equivalent**, modulo analyticity assumption for Cauchy.

- Interpolation: for basic properties.
- JCF: for solving matrix equations (e.g., $X^2 = A$, $e^X = A$). For evaluation (normal A).
- Cauchy: various uses.

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Specific f

Can usually exploit f to beat direct use of above defs.

Some Matrix Functions Not Discussed Later

Function	Literature
exp	Huge, mostly low practical relevance
cos, sin	Small
A^D	Large, but not typically treated as $f(A)$
$A = UH$	Large

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$f(A)\,b$

- Compute $f(A)b$ without (explicitly) computing $f(A)$.
- Problem of particular interest for large, sparse A.
- Concentrate here on dense matrices—subproblem of sparse case when projection method used.

Lattice Quantum Chromodynamics (QCD)

Simulations with **overlap-Dirac operator** require soln of

$$\big(G - \mathrm{sign}(H)\big)x = b. \qquad (*)$$

- $G = \mathrm{diag}(\pm 1)$.
- H sparse, complex, Hermitian.
- $n \approx 10^6$.
- $H = Q\mathrm{diag}(\lambda_i)Q^*$ (spectral decomp) $\Rightarrow$ $\mathrm{sign}(H) = Q\mathrm{diag}(\mathrm{sign}(\lambda_i))Q^*$ (**dense!**).

Solve $(*)$ by Krylov methods $\Rightarrow$ need $\mathrm{sign}(H)c$ for given c.

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See Andreas Frommer: Thursday, 12 pm

Computing $\mathrm{sign}(A)v$ with Applications in QCD

Differential Equations

For $y \in \mathbb{C}^n$, $A \in \mathbb{C}^{n\times n}$,

$$\frac{dy}{dt} = Ay + f(t,y), \qquad y(0) = c,$$

has solution

$$y(t) = e^{At}c + \int_0^t e^{A(t-s)} f(s,y)\,ds.$$

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- Hochbruck, Lubich & Selhofer. Exponential integrators for large systems of differential equations. *SISC*, 1998.
- Cox & Matthews. Exponential time differencing for stiff systems. *J. Comput. Phys.*, 2002.
- Kassam & Trefethen. Fourth-order time-stepping for stiff PDEs. *SISC*, 2005.

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See M. Hönig: Thursday, 12.30 pm

Regularization of inverse problems by exponential integrators

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See also Minisymposium 23, Wednesday 2.15pm

Applied Linear Algebra & Differential Equations (organizer: A. Ostermann)

Interpolation

If A has *distinct eigenvalues* λ_j, **Lagrange** interp poly:

$$f(A)b = \sum_{j=0}^{n} f_j \ell_j(A)b, \qquad \ell_j(x) = \frac{\displaystyle\prod_{k=0,\ k\neq j}^{n} (x-\lambda_k)}{\displaystyle\prod_{k=0,\ k\neq j}^{n} (\lambda_j-\lambda_k)}.$$

Cost: $O(n^4)$ flops. (Barycentric form "singular".)
For any A, **Newton** divided difference form:

$$f(A)b = \sum_{i=0}^{n} c_i \prod_{j=0}^{i-1} (A-\lambda_j I)b, \qquad c_i = \text{(confluent) div. diffs.}$$

Requires derivatives of f. Cost: $O(n^3)$ flops.

Cauchy Integral Theorem

$$y = \frac{1}{2\pi i}\int_\Gamma f(z)(zI - A)^{-1} b\, dz =: \int_\Gamma g(z)\, dz.$$

Issues:

- Choice of contour Γ.
- Take into account singularities/branch points.
- (Conformal) transformation.
- Assumptions on A.
- Choice of quadrature rule.
- Number of quadrature points.
- Error bounds.

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Generic implementation (e.g. contour = circle) doesn't work well in general.

More on Cauchy

See Nick Trefethen: Wed 11.30 am

Talbot Quadratures and Rational Approximations

See Michiel Hochstenbach: Wed 12.00 pm

Subspace Extraction for Matrix Functions

$\log(A)\, b$

Definition

$A \in \mathbb{C}^{n\times n}$ with no eigenvalues on $\mathbb{R}^-$.
$X = \log A$ denotes unique X such that

- $e^X = A$.
- $-\pi < \operatorname{Im}\big(\lambda(X)\big) < \pi$.

Wouk (1965):

$$\log A = \int_0^1 (A - I)\big[t(A - I) + I\big]^{-1}\, dt.$$

Apply quad. rule $\displaystyle\int_0^1 f(t)\, dt \approx \sum_{k=1}^{m} c_k f(t_k)$.

$\log(A)\,b$

Combine with **Hessenberg reduction** $A = QHQ^T$ to get

$$(\log A)\,b \approx Q \sum_{k=1}^{m} c_k \left[t_k(H - I) + I\right]^{-1} d, \qquad d = Q^T(A - I)b,$$

Costs $(10/3)n^3 + 2mn^2$ flops.

- When $\|I - A\| < 1$ can use m-point **Gauss-Legendre** $\equiv$ **Padé approximation** (Dieci, Morini & Papini, 1996). Choose m using (Kenney & Laub, 2001)

$$\|r_{mm}(X) - \log(I + X)\| \le |r_{mm}(-\|X\|) - \log(1 - \|X\|)|. \quad (*)$$

- When $\|I - A\| > 1$ use adaptive quadrature.

Experiments (1)

$A =$ `eye(64)` $+ 0.9$ `urandn(64)`, $b =$ `urandn(64,1)`.

$$\|I - A\|_2 = 0.9,\ \|\log A\|_2 = 1.0.$$

	Adaptive quad.		Gauss-Legendre		
tol	g evals	abs err	m	abs err	Upper bound $(*)$
1e-3	18	5.6e-10	7	9.7e-13	3.2e-4
1e-6	18	5.6e-10	12	3.1e-15	4.7e-7
1e-9	18	5.6e-10	17	3.1e-15	6.8e-10

Experiments (2)

$A =$ `gallery('parter',64)`, $b =$ `urandn(64,1)`.

$\|I - A\|_2 = 3.2$, $\|\log A\|_2 = 1.9$.

	Adaptive quad.		Gauss-Legendre	
tol	g evals	abs err	m	abs err
1e-3	48	1.6e-4	8	5.2e-6
1e-6	48	1.4e-10	10	2.5e-7
1e-9	138	1.6e-13	14	5.2e-10

$A^\alpha\, b$ via ODE IVP

Definition

$A^\alpha = \exp(\alpha \log A)$, $\alpha \in \mathbb{R}$.

$$\frac{dy}{dt} = \alpha(A - I)\big[t(A - I) + I\big]^{-1} y, \qquad y(0) = b$$

has unique solution

$$y(t) = \big[t(A - I) + I\big]^\alpha b$$

so

$$y(1) = A^\alpha b.$$

Used by Allen, Baglama & Boyd (2000) for $\alpha = 1/2$, spd A.

Experiment

With MATLAB's `ode45`.

$A =$ `gallery('parter',64)`, $b =$ `randn(64,1)`.

$f(A)$	tol	Succ steps	Fail atts	f evals	Rel err
$A^{-1/2}$	1e-3	12	0	73	3.5e-8
	1e-6	14	0	85	6.0e-9
	1e-9	40	0	241	7.7e-12
$A^{2/5}$	1e-3	15	0	79	2.8e-8
	1e-6	16	0	91	2.4e-9
	1e-9	54	0	325	1.8e-12

$A^\alpha\, b$ via Binomial Expansion

Write $A = s(I - C)$ and choose s to minimize $\rho(C)$:

- $s = (\lambda_{\min} + \lambda_{\max})/2$ if $\lambda_i > 0$.
- $s = \mathrm{trace}(A^*A)/\mathrm{trace}(A^*)$ minimizes $\|C\|_F$.

$$(I - C)^\alpha = \sum_{j=0}^{\infty} \binom{\alpha}{j} (-C)^j, \qquad \rho(C) < 1.$$

So

$$A^\alpha b = s^\alpha \sum_{j=0}^{\infty} \binom{\alpha}{j} (-C)^j b.$$

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$$A^\alpha b = s^\alpha \sum_{j=0}^{\infty} \binom{\alpha}{j} (-C)^j b.$$

For M-matrices, required splitting with $C \geq 0$ always exists.

Summary

Tools for $f(A)\,b$ include

- quadrature
- approximation (Padé, best L_∞)
- partial fraction expansions
- numerical solution of ODE IVP
- power series.

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Much scope for further work!

References

- Philip I. Davies and Nicholas J. Higham.
  Computing $f(A)b$ for matrix functions f.
  In Artan Boriçi, Andreas Frommer, Báalint Joó, Anthony Kennedy, and Brian Pendleton, editors, *QCD and Numerical Analysis III*, volume 47 of *Lecture Notes in Computational Science and Engineering*, pages 15–24. Springer-Verlag, Berlin, 2005.

- Nicholas J. Higham.
  Functions of a Matrix: Theory and Computation.
  Book in preparation.